

Quasi-two-dimensional bound states

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(Dated: July 3, 2012)

We consider the problem of N identical fermions of mass m_{\uparrow} and one distinguishable particle of mass m_{\downarrow} interacting via short-range interactions in a confined quasi-two-dimensional (quasi-2D) geometry. For $N = 2$ and mass ratios $m_{\uparrow}/m_{\downarrow} < 13.6$, we find non-Efimov trimers that smoothly evolve from 2D to 3D. In the limit of strong 2D confinement, we show that the energy of the $N + 1$ system can be approximated by an effective two-channel model. We use this approximation to solve the $3 + 1$ problem and we find that a bound tetramer can exist for mass ratios $m_{\uparrow}/m_{\downarrow}$ as low as 5 for strong confinement, thus providing the first example of a universal, non-Efimov tetramer involving three identical fermions.

An understanding of the few-body problem can be important for gaining insight into the many-body system. In dimensions higher than one, few-body bound states can, for instance, impact the statistics of the many-body quasiparticle excitations. Indeed, for fermionic systems, the two-body bound state is fundamental to the understanding of the BCS-BEC crossover [1–4], while the existence of three-body bound states of fermions [5, 6] with unequal masses can lead to dressed trimer quasiparticles in the highly polarized Fermi gas [7]. Even in one dimension (1D), few-body bound states can impact the many-body phase: It has already been shown that one can have a Luttinger liquid of trimers [8].

In general, attractively interacting bosons readily form bound clusters, with the celebrated example being the Efimov effect in 3D [9], where there is a universal hierarchy of trimer states for resonant short-range interactions. However, for identical fermions it is less clear whether bound states exist, since these are constrained to have odd angular momentum owing to Pauli exclusion. For short-range interactions in 3D, trimers consisting of two identical fermions with mass m_{\uparrow} and one distinguishable particle with mass m_{\downarrow} can only exist above the critical mass ratio $m_{\uparrow}/m_{\downarrow} \simeq 8.2$ [5], while Efimov trimers only appear once $m_{\uparrow}/m_{\downarrow} \gtrsim 13.6$ [10]. However, the existence of larger $(N+1)$ -body bound states involving $N > 2$ identical fermions remains largely unknown — it has only recently been shown that Efimov tetramers exist in 3D [11].

In this Letter, we investigate the problem of N identical fermions interacting with one distinguishable particle in a confined quasi-2D geometry, where the centrifugal barrier is reduced and the binding of fermions should be favored. Such 2D geometries have recently been realised in ultracold atomic Fermi gases [12–16], where the fermions are confined to 2D with an effective harmonic potential. In addition to allowing one to explore the 2D-3D crossover, the harmonic confinement can strongly modify the scattering properties of atoms via confinement-induced resonances [6, 17, 18]. It has already been demonstrated that stable non-Efimov trimers can exist for lower mass ratios $m_{\uparrow}/m_{\downarrow}$ in quasi-2D [6, 19].

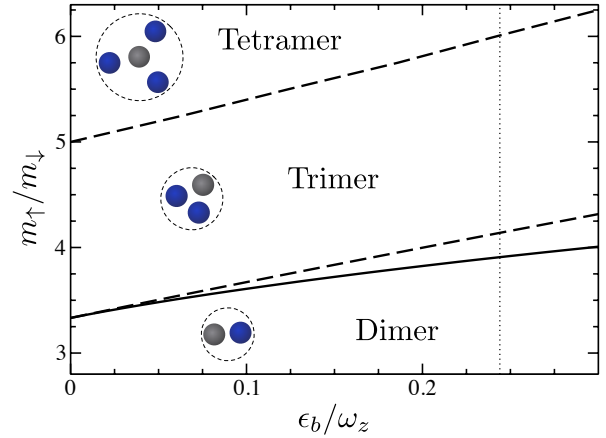


FIG. 1: (Color online) Critical mass ratio for the appearance of trimers and tetramers in quasi-2D, where the 2D limit corresponds to $\epsilon_b/\omega_z \rightarrow 0$. The solid line follows from the solution of the full three-body quasi-2D problem, Eq. (8). Dashed lines follow from an effective two-channel model. The vertical dotted line marks unitarity, where the 3D scattering length diverges.

Here we show that tetramers involving $N = 3$ identical fermions can appear for $m_{\uparrow}/m_{\downarrow}$ as low as 5 in quasi-2D (see Fig. 1), thus putting it within reach of current cold-atom experiments.

We construct the general equations for the bound state of the $N + 1$ system in quasi-2D and we reveal how to simplify the problem in the case of the trimer ($N = 2$). In the limit of strong 2D confinement, we show that the $N + 1$ problem can be described by an effective two-channel model, analogous to that used for Feshbach resonances. This important simplification allows us to solve the aforementioned $N = 3$ problem in quasi-2D.

In the following, we assume the two atomic species $\{\uparrow, \downarrow\}$ to be confined to a quasi-2D geometry by an approximately harmonic potential along the z direction, $V_{\uparrow, \downarrow}(z) = \frac{1}{2}m_{\uparrow, \downarrow}\omega_z^2 z^2$. Here, we restrict ourselves to equal confinement frequencies for the two species since it allows a separation of the relative and center of mass motion

along the z -direction, as we discuss below. Such a scenario can, in principle, be engineered experimentally using spin-dependent optical lattices. However, even in the case where the confinement frequency is species dependent, regimes exist in which the few-body properties are only weakly affected by this dependence. For instance, for large mass ratios and on the molecular side of the Feshbach resonance, once the $\uparrow\downarrow$ dimer is smaller than the light atom oscillator length, $l_z^\downarrow = \sqrt{\hbar/m_\downarrow\omega_z}$, the light atom is essentially confined by its interaction with the heavy atoms [6].

The starting point of our analysis is the T -matrix describing the repeated two-body interspecies interaction. In the ultracold gases, the interaction is described by a zero-range model as the van der Waals range of the interatomic potential is much smaller than all other length scales in the problem, including the confinement lengths. The T -matrix may be considered in the basis of the individual motion of a spin- \downarrow and \uparrow atom. However, due to the restriction to equal confinement frequencies for the two species, the center of mass and relative motion separates and it is advantageous to work in this basis. In the center of mass frame of the harmonic oscillator potential, at energy ϵ below the two-body threshold ω_z (we set $\hbar = 1$) and at total 2D momentum \mathbf{q} , the T -matrix takes the form [20]

$$\mathcal{T}(\mathbf{q}, \epsilon) = \frac{\sqrt{2\pi}}{m_r} \left\{ \frac{l_z^r}{a_s} - \mathcal{F} \left(\frac{-\epsilon + \mathbf{q}^2/2(m_\uparrow + m_\downarrow)}{\omega_z} \right) \right\}^{-1}, \quad (1)$$

where the zero-range interaction is renormalized by the use of the 3D scattering length, a_s . Here, $m_r = m_\uparrow m_\downarrow / (m_\uparrow + m_\downarrow)$ is the reduced mass and $l_z^r = \sqrt{1/2m_r\omega_z}$ is the confinement length corresponding to the relative motion. We use the definition of \mathcal{F} [21]

$$\mathcal{F}(x) = \int_0^\infty \frac{du}{\sqrt{4\pi u^3}} \left(1 - \frac{e^{-xu}}{\sqrt{[1 - \exp(-2u)]/2u}} \right). \quad (2)$$

The two-dimensional scattering always admits a two-body bound state of mass $M = m_\uparrow + m_\downarrow$ and binding energy $\epsilon_b > 0$ satisfying $l_z^r/a_s = \mathcal{F}(\epsilon_b/\omega_z)$.

The T -matrix in the basis of individual motion is related to \mathcal{T} by the change of basis

$$T_{n_0 n_1}^{n'_0 n'_1}(\mathbf{q}, \epsilon) = \sum_{n, n_r, n'_r} C_{nn_r}^{n_0 n_1}(m_\downarrow, m_\uparrow) C_{nn'_r}^{n'_0 n'_1}(m_\downarrow, m_\uparrow) \times \psi_{n_r}(0) \psi_{n'_r}(0) \mathcal{T}(\mathbf{q}, \epsilon - n\omega_z). \quad (3)$$

Here, n_0 and n_1 are the quantum numbers labelling the eigenstates of the single-particle Hamiltonians $\mathcal{H}_{\downarrow, \uparrow} = -\frac{\nabla_{0,1}^2}{2m_{\downarrow, \uparrow}} + \frac{1}{2}m_{\downarrow, \uparrow}\omega_z^2 z_{0,1}^2$ while n_r and n are the quantum numbers in the basis of relative, $z_{01} = z_0 - z_1$, and center of mass, $Z_{01} = (m_\downarrow z_0 + m_\uparrow z_1)/M$, coordinates. The wavefunction of the relative motion takes the value $\psi_{n_r}(0) = (-1)^{n_r/2} \sqrt{(n_r - 1)!/n_r!}$ if n_r is

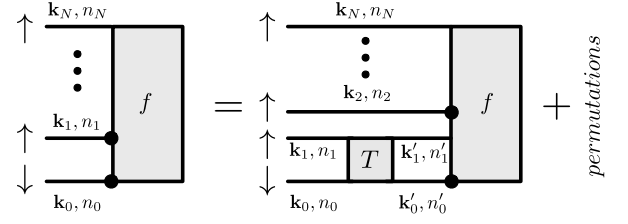


FIG. 2: The diagrams which give the binding energy of the $N + 1$ bound state in quasi-2D. Black dots indicate the initial interaction inside f .

even, and 0 otherwise. The Clebsch-Gordan coefficients $C_{nn_r}^{n_0 n_1}(m_\downarrow, m_\uparrow) \equiv \langle n_0 n_1 | n n_r \rangle$ were obtained in Ref. [22] and vanish unless $n_0 + n_1 = n + n_r$.

We now turn to the question of the existence of bound states consisting of N spin- \uparrow atoms and a single spin- \downarrow atom. To this end, we construct the sum of connected diagrams with $N + 1$ incoming atoms (Fig. 2). The \uparrow atoms are considered on-shell with 2D momenta \mathbf{k}_i , harmonic oscillator quantum numbers n_i , and corresponding single-particle energies $\epsilon_{\mathbf{k}_i n_i \uparrow} = k_i^2/2m_\uparrow + n_i\omega_z$ for $i = 1, \dots, N$. We consider scattering in the centre of mass frame of the 2D motion and at a total energy E below the $N + 1$ atom threshold $(N + 1)\omega_z/2$. Thus, the \downarrow atom has 2D momentum $\mathbf{k}_0 \equiv -\sum_{i=1}^N \mathbf{k}_i$, harmonic oscillator quantum number n_0 , and energy $E_0 \equiv E - \sum_{i=1}^N \epsilon_{\mathbf{k}_i n_i \uparrow}$. The sum of diagrams with $N + 1$ incoming particles in which the \downarrow atom interacts first with the \uparrow atom numbered 1 is denoted $f_{\mathbf{k}_2 \dots \mathbf{k}_N}^{n_0 \dots n_N}$. Note that there is no dependence on \mathbf{k}_1 as the initial interaction depends only on the total momentum of the two atoms.

The occurrence of a bound state corresponds to a singularity of f at its binding energy. This singularity results from the summation of an infinite number of diagrams and, at the pole, f satisfies the homogeneous integral equation illustrated in Fig. 2: The initial interaction is described by a T -matrix, and then the spin- \downarrow atom subsequently interacts with another of the \uparrow atoms. Thus, the right hand side contains $N - 1$ terms and the integral equation satisfied by the bound state energy is (setting the volume to 1):

$$f_{\mathbf{k}_2 \dots \mathbf{k}_N}^{n_0 \dots n_N} = - \sum_{\mathbf{k}'_1, n'_0, n'_1} \frac{T_{n_0 n_1}^{n'_0 n'_1}(\mathbf{k}_0 + \mathbf{k}_1, E_0 + \epsilon_{\mathbf{k}_1 n_1 \uparrow})}{E_0 + \epsilon_{\mathbf{k}_1 n_1 \uparrow} - \epsilon_{\mathbf{k}'_0 n'_0 \downarrow} - \epsilon_{\mathbf{k}'_1 n'_1 \uparrow}} \times \left\{ f_{\mathbf{k}'_1 \mathbf{k}_3 \dots \mathbf{k}_N}^{n'_0 n'_1 n_3 \dots n_N} + \dots + f_{\mathbf{k}_2 \dots \mathbf{k}_{N-1} \mathbf{k}'_1}^{n'_0 n_N n_2 \dots n_{N-1} n'_1} \right\}, \quad (4)$$

where $\mathbf{k}'_0 = \mathbf{k}_0 + \mathbf{k}_1 - \mathbf{k}'_1$, and the minus sign on the *r.h.s.* appears because f is antisymmetric under the exchange of incoming fermions. Equation (4) embodies a simple and generic formulation for the $(N + 1)$ -body problem in quasi-2D, which in principle allows us to capture the crossover from 2D to 3D. Indeed, for the case of $N = 2$, it is a generalization of the Skorniakov-Ter-Martirosian

equation for atom-dimer scattering [23], while for $N = 1$, Eq. (4) simply reduces to the condition for the two-body binding energy. Finally, we note that Ref. [24] derived an expression similar to our Eq. (4) for the 3D $N + 1$ problem.

An important simplification to Eq. (4) becomes possible in the limit of strong quasi-2D confinement, $\omega_z \gg \epsilon_b$. Here, the function \mathcal{F} can be expanded as

$$\mathcal{F}(x) \approx \frac{1}{\sqrt{2\pi}} \ln(\pi x/B) + \frac{\ln 2}{\sqrt{2\pi}} x + \mathcal{O}(x^2) \quad (5)$$

with $B \approx 0.905$ [20, 21]. On the other hand, consider the denominator on the *r.h.s.* of Eq. (4) which we shall write for simplicity as $\epsilon - n\omega_z$. Here, the typical energy scale $\epsilon \sim \epsilon_b$ since, for bound states, the function f is strongly peaked at momenta $\sim \sqrt{2m_r\epsilon_b}$, while it quickly decays for large momenta. Now, if we expand the denominator in powers of ϵ_b/ω_z (assuming $n \neq 0$), then the lowest order term vanishes when integrated over momentum due to the antisymmetry of $f_{\mathbf{k}_1' \dots}$. Consequently, the lowest non-vanishing contribution from the denominator is of order $(\epsilon_b/\omega_z)^2$ when the harmonic oscillator index n is non-zero. We conclude that to linear order in ϵ_b/ω_z the integral equation for the $N + 1$ bound state reduces to

$$\begin{aligned} f_{\mathbf{k}_2 \dots \mathbf{k}_N} &= \tilde{T}(\mathbf{k}_0 + \mathbf{k}_1, \tilde{E}_0 + \epsilon_{\mathbf{k}_1 \uparrow}) \\ &\times \sum_{\mathbf{k}_1'} \frac{f_{\mathbf{k}_1' \mathbf{k}_3 \dots \mathbf{k}_N} + \dots + f_{\mathbf{k}_2 \dots \mathbf{k}_{N-1} \mathbf{k}_1'}}{\tilde{E}_0 + \epsilon_{\mathbf{k}_1 \uparrow} - \epsilon_{\mathbf{k}_0 \downarrow} - \epsilon_{\mathbf{k}_1' \uparrow}}, \quad (6) \end{aligned}$$

with the single particle energies $\epsilon_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}0}$, $\tilde{E}_0 = E - \sum_{i=1}^N \epsilon_{\mathbf{k}_i \uparrow}$, and \tilde{T} obtained from Eq. (1) using the linear expansion of \mathcal{F} , Eq. (5). As the effects of confinement in this limit are contained solely within the linearized T -matrix, Eq. (6) may be obtained through a strictly 2D 2-channel model [25], where the closed channel corresponds to excited harmonic oscillator modes. Thus, the confinement length l_z^r plays the role of an effective range in this model, with the 2D limit $l_z^r/a_s \rightarrow 0$ corresponding to a single-channel model. This simplification crucially depends on the antisymmetry resulting from Fermi statistics and it thus does not apply to bound clusters involving bosons confined to 2D, as considered in Refs. [26, 27]. Finally, we note that a similar simplification was recently obtained for quasi-1D atom-dimer scattering [28].

We now proceed to solve the three-body problem using the above methods. First, note that using the zero-range condition and removing the center of mass generally allows one to reduce the number of harmonic oscillator quantum numbers by two in Eq. (4) [6]. For the three-body problem, this is achieved by changing coordinates to the relative motion of the two atoms initially interacting, $z_{01} = z_0 - z_1$, the relative motion of the pair and the third atom, $z_2^{01} = (m_\downarrow z_0 + m_\uparrow z_1)/(m_\downarrow + m_\uparrow) - z_2$, and the center of mass $Z_{012} = (m_\downarrow z_0 + m_\uparrow z_1 + m_\uparrow z_2)/(m_\downarrow + 2m_\uparrow)$. Defining the corresponding quantum numbers n_{01} , n_2^{01} ,

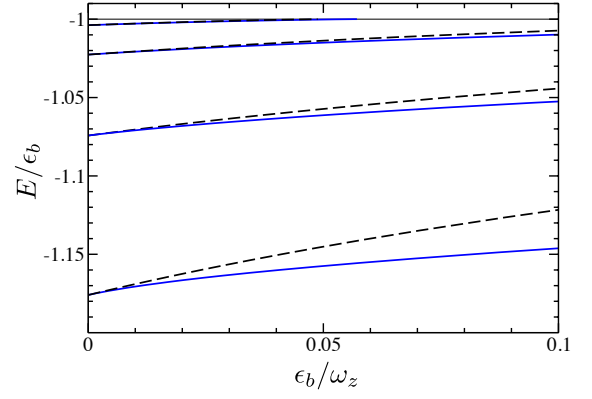


FIG. 3: (Color online) Energy of the trimer in quasi-2D for mass ratios $m_\uparrow/m_\downarrow = 3.5, 4, 5, 6.64$ (from top to bottom). The solid lines correspond to the full calculation, while the dashed lines are derived from the effective two-channel model, Eq. (6).

and N_{012} , we adopt the new basis:

$$\chi_{\mathbf{k}_2}^{n_2^{01}} = \frac{1}{\psi_{n_{01}}(0)} \sum_{n_0 n_1 n_2} \langle N_{012} n_2^{01} n_{01} | n_0 n_1 n_2 \rangle f_{\mathbf{k}_2}^{n_0 n_1 n_2}. \quad (7)$$

Here, we have dropped n_{01} from the *l.h.s.* as the resulting equation will be independent of this index. Also, the center of mass quantum number, N_{012} , has been neglected as it only causes a shift in the energy; since we consider the lowest lying trimer, N_{012} will be set to 0 in the following. In the new basis, Eq. (4) for the trimer becomes

$$\begin{aligned} \chi_{\mathbf{k}_2}^{n_2^{01}} &= \mathcal{T}(\mathbf{k}_2, E - \epsilon_{\mathbf{k}_2 \uparrow} - n_2^{01} \omega_z) \\ &\times \sum_{\mathbf{k}_1', n_1^{02} n_{02} n_{01}} \frac{\psi_{n_{02}}(0) \psi_{n_{01}}'(0) \langle n_2^{01} n_{01}' | n_1^{02} n_{02} \rangle \chi_{\mathbf{k}_1'}^{n_1^{02}}}{E - \epsilon_{\mathbf{k}_1' \uparrow} - \epsilon_{\mathbf{k}_2 \uparrow} - \epsilon_{\mathbf{k}_1' + \mathbf{k}_2 \downarrow} - (n_1^{02} + n_{02}) \omega_z}, \quad (8) \end{aligned}$$

where we can see that the *r.h.s.* indeed does not depend on n_{01} . The matrix element in Eq. (8) may be evaluated by a series of coordinate transformations:

$$\begin{aligned} \langle n_2^{01} n_{01} | n_1^{02} n_{02} \rangle &= \sum_{n_0 n_1 n_2 N_{01} N_{02}} C_{0n_2^{01}}^{N_{01} n_2}(M, m_\uparrow) \\ &\times C_{N_{01} n_{01}}^{n_0 n_1}(m_\downarrow, m_\uparrow) C_{N_{02} n_{02}}^{n_0 n_2}(m_\downarrow, m_\uparrow) C_{0n_1^{02}}^{N_{02} n_1}(M, m_\uparrow), \end{aligned}$$

where several sums can be dropped due to the constraints on the Clebsch-Gordan coefficients.

Since the trimer consists of identical fermions, it must necessarily have odd angular momentum L in the x - y plane of the 2D layer. Thus, the lowest-energy trimer has $L = 1$, and it can be regarded as a p -wave pairing of \uparrow fermions mediated by their s -wave interactions with the light \downarrow particle. In this case, we have $\chi_{\mathbf{k}_2}^{n_2^{01}} = \tilde{\chi}_{k_2}^{n_2^{01}} e^{i\phi_2}$, where ϕ_2 is the angle of \mathbf{k}_2 with respect to the x -axis and $\tilde{\chi}$ is a function of $k_2 \equiv |\mathbf{k}_2|$. Integrating over ϕ_2 in Eq. (8) then leaves an integral equation that only depends on k_2

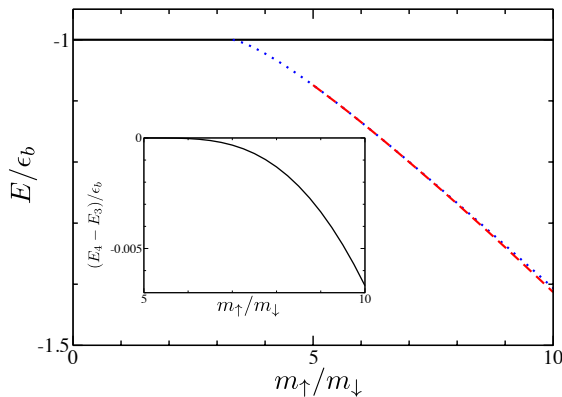


FIG. 4: (Color online) Energy of the dimer (solid line), trimer (dotted), and quadrumer (dashed) in 2D as a function of mass ratio. The trimer binds when $m_{\uparrow}/m_{\downarrow} > 3.33$, consistent with Ref. [19], while the trimer-tetramer transition occurs at $m_{\uparrow}/m_{\downarrow} = 5.0$. Inset: The difference between trimer and quadrumer energies, $E_3 - E_4$.

and n_2^{01} . The same applies for the two-channel model Eq. (6) with $N = 2$, where now there is only a dependence on k_2 .

We have calculated the trimer binding energy as a function of confinement for a range of mass ratios, as depicted in Fig. 3. We see that the binding energy decreases as we perturb away from 2D and the centrifugal barrier is increased. Correspondingly, we find that the critical mass ratio $m_{\uparrow}/m_{\downarrow}$ for trimer binding smoothly evolves from the 2D limit of 3.33 [19] towards the 3D result of 8.2 [5], as shown in Fig. 1. For the special case of ${}^6\text{Li}$ - ${}^{40}\text{K}$ mixtures, where $m_{\uparrow}/m_{\downarrow} = 6.64$, our results agree with Ref. [6]. In the limit of strong 2D confinement, we see that the two-channel model captures the lowest-order dependence on ϵ_b/ω_z of the trimer energy and critical mass ratio.

We can exploit the two-channel model (6) to solve the more complicated four-body ($N = 3$) problem in quasi-2D. Once again, the presence of identical fermions requires us to consider total angular momentum $L = 1$. Thus, we have for the tetramer

$$f_{\mathbf{k}_2\mathbf{k}_3} = \tilde{f}(k_2, k_3, \Delta\phi_{32})e^{i\phi_2} = -\tilde{f}(k_3, k_2, -\Delta\phi_{32})e^{i\phi_3},$$

where $\Delta\phi_{32} = \phi_3 - \phi_2$. We note that a similar equation for the tetramer energy was obtained for the 3D problem in Ref. [11].

Beginning with the 2D limit ($\epsilon_b/\omega_z = 0$), we determine the energy of the tetramer compared to the trimer and dimer energies (see Fig. 4). Following the transition from a dimer to a trimer at mass ratio $m_{\uparrow}/m_{\downarrow} \simeq 3.33$, we find a trimer-tetramer transition at $m_{\uparrow}/m_{\downarrow} \simeq 5.0$. In principle, we can use Eq. (4) to consider bound states of even larger N , but the problem quickly becomes intractable numerically for $N > 3$. However, we conjecture that composite bound states of larger N become possible as $m_{\uparrow}/m_{\downarrow}$ is increased, since the relative importance of the centrifugal

barrier between heavy particles (which goes as $1/m_{\uparrow}$) diminishes compared with the effective attractive potential induced by the light particle ($\sim 1/m_{\downarrow}$).

Perturbing away from the 2D limit, we find that the trimer-tetramer transition shifts to larger $m_{\uparrow}/m_{\downarrow}$ with increasing ϵ_b/ω_z , as shown in Fig. 1. Eventually, we expect to encounter the four-body Efimov effect in 3D for $m_{\uparrow}/m_{\downarrow} > 13.4$ [11]. However, it remains an open question whether our quasi-2D tetramers exist in 3D below the critical mass ratio for Efimov physics.

To conclude, we have provided the first example of a universal, non-Efimov tetramer involving three identical fermions. Since this quasi-2D tetramer exists for mass ratios $m_{\uparrow}/m_{\downarrow}$ as low as 5, it could potentially be probed with ultracold ${}^6\text{Li}$ - ${}^{40}\text{K}$ mixtures. Its small binding energy (Fig. 4) suggests that it could appear as a resonance in atom-trimer interactions. For instance, if a cloud of trimers were prepared under strong quasi-2D confinement, signatures of the resonance could be observed by colliding a cloud of heavy atoms with a cloud of trimers, similar to the proposal of Ref. [29] for detecting an atom-dimer resonance. In addition, the presence of trimers and tetramers has implications for the many-body phases in quasi-2D, particularly for the highly polarized Fermi gas [30, 31].

We emphasize that although we have focussed on the $N + 1$ problem in quasi-2D, the form of Eq. (4) is completely general and may be extended to other shapes of the confining potential and/or different dimensionalities. For instance, in quasi-1D one would use the T -matrix derived in Refs. [17, 21], along with appropriately redefined harmonic oscillator and momentum indices. Furthermore, the problem may be studied close to narrow Feshbach resonances, characterized by a large effective range, by using an energy-dependent scattering length [32]. Finally, our work suggests that a two-channel model may be used to model strongly confined quasi-2D Fermi systems in general.

We gratefully acknowledge fruitful discussions with Stefan Baur, Andrea Fischer, Pietro Massignan, Wave Ngampruetikorn, and Dmitry Petrov. MMP acknowledges support from the EPSRC under Grant No. EP/H00369X/1. JL acknowledges support from a Marie Curie Intra European grant within the 7th European Community Framework Programme.

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